

ABSTRACT OF THE DISCLOSURE

A computer based system for analyzing a set of data objects and establishing a mechanism model representing a set of features that is likely to correlate with a specified response characteristic. A computer may establish a description for each of the data objects
5 based on a comparison between a set of descriptors and features of the data objects. The computer may then select a group of the data objects that have similar descriptions and that represent the specified response characteristic. The computer may then adaptively learn a mechanism model by mapping the discriminating features of the group back to the objects in the group. The computer may further designate the mechanism model as a new descriptor and
10 iteratively repeat the process to establish yet an improved mechanism model. The invention is particularly well suited for use in establishing pharmacophores representing chemical structures that are likely to correlate with activity in a particular assay.